Amendments to the Claims

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims

1. (previously presented) A method of selecting an odorant or two or more odorants for a perfumed product, comprising the following steps in sequence:

   (a) for one group of odorants, determining a parameter from the relative concentration of an odorant in the phase to be perfumed relative to the concentration in the perfumed phase;

   (b) determining the descriptors of odorants using a mathematical method;

   (c) imputing the parameters determined in step (a) into a determination model and carrying out a regression calculation;

   (d) calculating a prediction for all calculated odorants based on the regression calculation; and

   (e) using the odorants most effective according to the prediction in the composition of a perfume oil.

2. (previously presented) A method according to Claim 1, wherein the determination of the relative distribution of odorants is carried out by analysis of the concentration in the perfumed phase and the phase to be perfumed.

3. (previously presented) A method according to Claim 1, wherein the partition equilibrium between the gas phase and a liquid phase is determined.

4. (previously presented) A method according to Claim 1, wherein the partition equilibrium between the gas phase and a solid phase is determined.

5. (previously presented) A method according to Claim 1, wherein the partition equilibrium between a liquid phase and a solid phase is determined.

6. (previously presented) A method according to Claim 1, wherein the partition equilibrium between two liquid phases is determined.

7. (previously presented) A method according to Claim 1, wherein the group of odorants comprises 2 to 200 individual compounds.

8. (previously presented) A method according to Claim 7, wherein the group of odorants comprises 10 to 100 individual compounds.

9. (previously presented) A method according to Claim 8, wherein the group of odorants comprises 20 to 50 individual compounds.

10. (previously presented) A method according to Claim 1, wherein, during the calculation of the descriptors of the odorants using a mathematical method, the following steps in sequence are performed:

(a) generating conformers;
(b) optimizing the field of force;
(c) selecting the conformers by accumulation analysis;
(d) performing a semi-empirical structure optimization;
(e) selecting further conformers by accumulation analysis;
(f) optimizing the structure using ab-initio or DFT calculations; and
(g) carrying out a COSMO-RS calculation.

11. (previously presented) A method according to Claim 1, wherein a dielectric continuum calculating method is used to calculated descriptors of the odorants.

12. (currently amended) A method according to Claim 1, wherein a mathematical determination model for the distribution between: (a) the gas phase and (b) a liquid or solid phase is described by the function

$$\log P^{X}_{gas,S} = C_{gen}\left(\mu^{X}_{gas} - \mu^{X}_{S}\right) + \text{const.}$$

$$= C_{gen}\,\mu^{X}_{gas} + C_S^0 M_0^X + C_S^2 M_2^X + C_S^3 M_3^X + C_S^4 M_4^X + C_S^{acc} M_{acc}^X + C_S^{don} M_{don}^X + \text{const.}$$

in which the symbols have the following meanings:
$P^{X}_{gas,S}$ represents a partition parameter between gas phase and liquid or solid phase;

c_{gen} represents a general, customized preliminary factor;

μ^X_{gas} represents the chemical potential of substance X in the gas phase according to COSMO-RS;

μ_S^X represents the chemical potential of substance X in the solid or liquid phase from regression;

const. represents the general regression constant;

c_S^i represents the expansion coefficient of the Taylor series from regression;

acc represents the hydrogen bridge acceptor;

don represents the hydrogen bridge donor; and

M_i^X represents the σ-moment of the i-th order of the substance X.

13. (currently amended) A method according to Claim 1, wherein a mathematical determination model for the distribution between: (a) a liquid or solid phase ~~on the one hand~~ and (b) a liquid or solid phase ~~on the other hand~~ is described by the function

$$\log P^X_{S,S'} = c_{gen}\left(\mu^X_S - \mu^X_{S'}\right) + const.$$
$$= c^0_{S,S'}M^X_0 + c^2_{S,S'}M^X_2 + c^3_{S,S'}M^X_3 + c^4_{S,S'}M^X_4 + c^{acc}_{S,S'}M^X_{acc} + c^{don}_{S,S'}M^X_{don} + const.$$

in which the symbols have the following meanings:

$P^x_{s,s'}$ represents the partition parameter between liquid phase S and liquid or solid phase S';

c_{gen} represents the general, customized preliminary factor;

μ^x_s represents the chemical potential of substance X in the liquid phase S according to COSMO-RS;

$\mu^x_{s'}$ represents the chemical potential of substance X in the solid or liquid phase S' from regression;

const represents the general regression constant;

c_s^i represents the expansion coefficient of the Taylor series from regression;
acc represents the hydrogen bridge acceptor;
don represents the hydrogen bridge donor; and
M_i^X represents the σ-moment of the i-th order of the substance X.

14. (previously presented) A method according to Claim 12, wherein a mathematical determination model is created using the σ-moments M_0^X, M_2^X, M_2^X, M_4^X, and M_{acc}^X, M_{don}^X and μ_{gas}^X as descriptors and a constant.

15. (previously presented) A method according to Claim 12, wherein a mathematical determination model is created using the σ-moments M_0^X, M_2^X, M_2^X, M_4^X, and M_{acc}^X, M_{don}^X and μ_{gas}^X as descriptors and a constant in combination with descriptors already known.

16. (previously presented) A method according to Claim 12, wherein a regression calculation is carried out to correlate the descriptors with the partition parameters of the odorants.

17. (previously presented) A method according to Claim 1, wherein a prediction is made for the partition parameters of odorants.

18. (previously presented) A method according to Claim 1, wherein the prediction of the partition parameters of

odorants is used for the composition of perfume oils and odorant mixtures.

19. (previously presented) A method according to Claim 1, wherein perfumed products are consumer products.

20. (previously presented) A method according to Claim 1, wherein perfumed products are detergents, care compositions, air fresheners and cleaners for industrial use.

21. (previously presented) A method according to Claim 1, wherein perfumed products are detergents, care compositions, air fresheners and cleaners in the domestic sector.

22. (previously presented) A method according to Claim 1, wherein perfumed products are detergents, care compositions, air fresheners and cleaners for veterinary use.

23. (previously presented) A method according to Claim 1, wherein perfumed products are detergents, care compositions, air fresheners and cleaners in body hygiene.

24. (withdrawn) Products containing perfumes which comprise odorants, wherein said odorants are selected for the products containing perfumes using a mathematical

determination model comprising the following steps in sequence:

(a) for one group of odorants, determining a parameter from the relative concentration of an odorant in the phase to be perfumed relative to the concentration in the perfumed phase;

(b) determining the descriptors of odorants using a mathematical method;

(c) imputing the parameters determined in step (a) into a determination model and carrying out a regression calculation;

(d) calculating a prediction for all calculated odorants based on the regression calculation; and

(e) using the odorants most effective according to the prediction in the composition of a perfume oil.

25. (withdrawn) Products according to Claim 24, wherein the odorant for the products containing perfumes are selected using a mathematical determination model which describes the distribution of odorants between a perfumed phase and a phase to be perfumed.

26. (withdrawn) Products according to Claim 24, wherein a dielectric continuum calculation method is used to calculate descriptors of the odorants.

27. (withdrawn) Products according to Claim 24, wherein the odorants for the perfumed products are selected using a

mathematical determination model in which the distribution between: (a) the gas phase and (b) a liquid or solid phase is calculated by the function

$$\log P^{X}_{gas,S} = C_{gen}\left(\mu^{X}_{gas} - \mu^{X}_{S}\right) + \text{const.}$$

$$= C_{gen}\mu^{X}_{gas} + C_S^0 M_0^X + C_S^2 M_2^X + C_S^3 M_3^X + C_S^4 M_4^X + C_S^{acc} M_{acc}^X + C_S^{don} M_{don}^X + \text{const.}$$

in which the symbols have the following meanings:

$P^{X}_{gas,S}$ represents a partition parameter between gas phase and liquid or solid phase;

c_{gen} represents a general, customized preliminary factor;

μ^{X}_{gas} represents the chemical potential of substance X in the gas phase according to COSMO-RS;

μ_S^X represents the chemical potential of substance X in the solid or liquid phase from regression;

const represents the general regression constant;

c_S^i represents the expansion coefficient of the Taylor series from regression;

acc represents the hydrogen bridge acceptor;

don represents the hydrogen bridge donor; and

M_i^X represents the σ-moment of the i-th order of the substance X.

28. (withdrawn) Products according to Claim 24, wherein the odorants for the products containing perfumes are selected using a mathematical determination model in which the distribution between: (a) a liquid or solid phase and (b) a liquid or solid phase is described by the function

$$\log P^{X}_{S,S'} = c_{gen}\left(\mu^{X}_{S} - \mu^{X}_{S'}\right) + const.$$
$$= c^{0}_{S,S'}M^{X}_{0} + c^{2}_{S,S'}M^{X}_{2} + c^{3}_{S,S'}M^{X}_{3} + c^{4}_{S,S'}M^{X}_{4} + c^{acc}_{S,S'}M^{X}_{acc} + c^{don}_{S,S'}M^{X}_{don} + const.$$

in which the symbols have the following meanings:

$P^{x}_{s,s'}$ represents the partition parameter between liquid phase S and liquid or solid phase S';

c_{gen} represents the general, customized preliminary factor;

μ^{x}_{s} represents the chemical potential of substance X in the liquid phase S according to COSMO-RS;

$\mu^{x}_{s'}$ represents the chemical potential of substance X in the solid or liquid phase S' from regression;

const represents the general regression constant;

c_{S}^{i} represents the expansion coefficient of the Taylor series from regression;

acc represents the hydrogen bridge acceptor;

don represents the hydrogen bridge donor; and

M_{i}^{X} represents the σ-moment of the i-th order of the substance X.

29. (withdrawn) Products according to Claim 27, wherein the odorants for the perfumed products are selected by means of a mathematical determination model using the σ-moments M_0^X, M_2^X, M_2^X, M_4^X, and M_{acc}^X, M_{don}^X and μ_{gas}^X as descriptors and a constant.

30. (withdrawn) Products according to Claim 27, wherein the odorants for the perfumed products are selected by means of a mathematical determination model using the σ-moments M_0^X,

M_2^X, M_2^X, M_4^X, and M_{acc}^X, M_{don}^X and μ_{gas}^X as descriptors and a constant in combination with descriptors already known.

31. (withdrawn) Products according to Claim 24, wherein said perfumed products are consumer products.

32. (withdrawn) Products according to Claim 24, wherein said products are detergents, care compositions, air fresheners and cleaners for industrial use.

33. (withdrawn) Products according to Claim 24, wherein said products are detergents, care compositions, air fresheners and cleaners in the domestic sector.

34. (withdrawn) Products according to Claim 24, wherein said ~~the~~ products are detergents, care compositions, air fresheners and cleaners for veterinary use.

35. (withdrawn) Products according to Claim 24, wherein said products are detergents, care compositions, air fresheners and cleaners for body hygiene.

36. (previously presented) A method of selecting an odorant or two or more odorants for the preparation of a perfume oil, comprising the following steps in sequence

(a) in a first step for one group of odorants, determining a parameter from the relative concentration of an odorant

in the phase to be perfumed relative to the concentration in the perfumed phase;

(b) determining the descriptors of odorants using a mathematical method;

(c) imputing the parameters determined in step (a) into a determination model and carrying out a regression calculation;

(d) making a prediction for all calculated odorants based on the regression calculation; and

(e) using the odorants most effective according to the prediction in the composition of a perfume oil.

37. (previously presented) A method according to Claim 36, wherein the determination of the relative distribution of odorants is carried out by analysis of the concentration in the perfumed phase and the phase to be perfumed.

38. (previously presented) A method according to Claim 36, wherein the partition equilibrium between the gas phase and a liquid phase is determined.

39. (previously presented) A method according to Claim 36, wherein the partition equilibrium between the gas phase and a solid phase is determined.

40. (previously presented) A method according to Claim 36, wherein the partition equilibrium between a liquid phase and a solid phase is determined.

41. (previously presented) A method according to Claim 36, wherein the partition equilibrium between the two liquid phases is determined.

42. (previously presented) A method according to Claim 36, wherein the group of odorants comprises 2 to 200 individual compounds.

43. (previously presented) A method according to Claim 42, wherein the group of odorants comprises 10 to 100 individual compounds.

44. (previously presented) A method according to Claim 43, wherein the group of odorants comprises 20 to 50 individual compounds.

45. (previously presented) A method according to Claim 36, wherein, in the calculation of the descriptors of the odorants using a mathematical method, the following steps in sequence are performed:

(a) generating conformers;
(b) optimizing the field of force;
(c) selecting the conformers by accumulation analysis;
(d) performing a semi-empirical structure optimization;
(e) selecting further conformers by accumulation analysis;
(f) optimizing the structure using ab-initio or DFT calculations; and
(g) carrying out a COSMO-RS calculation.

46. (previously presented) A method according to Claim 36, wherein a dielectric continuum calculating method is used to calculated descriptors of the odorants.

47. (currently amended) A method according to Claim 36, wherein a mathematical determination model for the distribution between: (a) the gas phase and (b) a liquid or solid phase is described by the function

$$\log P^{X}_{gas,S} = C_{gen}\left(\mu^{X}_{gas} - \mu^{X}_{S}\right) + \text{const.}$$

$$= C_{gen}\,\mu^{X}_{gas} + C_S^0 M_0^X + C_S^2 M_2^X + C_S^3 M_3^X + C_S^4 M_4^X + C_S^{acc} M_{acc}^X + C_S^{don} M_{don}^X + \text{const.}$$

in which the symbols have the following meanings:

$P^{X}_{gas,S}$ represents a partition parameter between gas phase and liquid or solid phase;

c_{gen} represents a general, customized preliminary factor;

μ^{X}_{gas} represents the chemical potential of substance X in the gas phase according to COSMO-RS;

μ_S^X represents the chemical potential of substance X in the solid or liquid phase from regression;

const represents the general regression constant;

c_S^i represents the expansion coefficient of the Taylor series from regression;

acc represents the hydrogen bridge acceptor;

don represents the hydrogen bridge donor; and

M_i^X represents the σ-moment of the i-th order of the substance X.

48. (currently amended) A method according to Claim 36, wherein a mathematical determination model for the distribution between: (a) a liquid or solid phase and (b) a liquid or solid phase is described by the function

$$\log P^{X}_{S,S'} = c_{gen}\left(\mu^{X}_{S} - \mu^{X}_{S'}\right) + const.$$
$$= c^{0}_{S,S'}M^{X}_{0} + c^{2}_{S,S'}M^{X}_{2} + c^{3}_{S,S'}M^{X}_{3} + c^{4}_{S,S'}M^{X}_{4} + c^{acc}_{S,S'}M^{X}_{acc} + c^{don}_{S,S'}M^{X}_{don} + const.$$

in which the symbols have the following meanings:

$P^{x}_{s,s'}$ represents the partition parameter between liquid phase S and liquid or solid phase S';

c_{gen} represents the general, customized preliminary factor;

μ^{x}_{s} represents the chemical potential of substance X in the liquid phase S according to COSMO-RS;

$\mu^{x}_{s'}$ represents the chemical potential of substance X in the solid or liquid phase S' from regression;

const represents the general regression constant;

c_{s}^{i} represents the expansion coefficient of the Taylor series from regression;

acc represents the hydrogen bridge acceptor;

don represents the hydrogen bridge donor; and

M_{i}^{X} represents the σ-moment of the i-th order of the substance X.

49. (previously presented) A method according to Claim 48, wherein a mathematical determination model is created using the σ-moments M_{0}^{X}, M_{2}^{X}, M_{2}^{X}, M_{4}^{X}, and M_{acc}^{X}, M_{don}^{X} and μ_{gas}^{X} as descriptors and a constant.

50. (previously presented) A method according to Claim 48, wherein a mathematical determination model is created using

the σ-moments M_0^x, M_2^x, M_2^x, M_4^x, and M_{acc}^x, M_{don}^x and μ_{gas}^x as descriptors and a constant in combination with descriptors already known.

51. (previously presented) A method according to Claim 36, wherein a regression calculation is carried out to correlate the descriptors with the partition parameters of the odorants.

52. (previously presented) A method according to Claim 36, wherein a prediction is made for the partition parameters of odorants.

53. (previously presented) A method according to Claim 36, wherein the prediction of the partition parameters of odorants is used for the composition of perfume oils and odorant mixtures.